WHAT IS CLAIMED IS:

1. A method of modeling the behavior of a molecule, comprising

selecting a torsion angle, rigid multibody model for said molecule, said model having equations of motion;

selecting an implicit integrator; and

generating an analytic Jacobian for said implicit integrator to integrate said equations of motion so as to obtain calculations of said behavior of said molecule.

2. The method of claim 1 wherein said analytic Jacobian is derived from an analytic Jacobian of the Residual Form of the equations of motion.

3. The method of claim 2 wherein said analytic Jacobian J comprises

$$J = \begin{pmatrix} \dfrac{\partial \dot{q}}{\partial q} & \dfrac{\partial \dot{q}}{\partial u} \\ \dfrac{\partial \dot{u}}{\partial q} & \dfrac{\partial \dot{u}}{\partial u} \end{pmatrix} \triangleq \begin{pmatrix} J_{qq} & J_{qu} \\ J_{uq} & J_{uu} \end{pmatrix}; \text{ and}$$

$$J_{qq} = \frac{\partial \dot{q}}{\partial q} = \frac{\partial (Wu)}{\partial q} \quad \text{and} \quad J_{qu} = \frac{\partial \dot{q}}{\partial u} = W$$

$$J_{uq} = \frac{\partial \dot{u}}{\partial q} = -M^{-1}\frac{\partial \rho_u(q,u,z)}{\partial q} \quad \text{and} \quad J_{uu} = \frac{\partial \dot{u}}{\partial u} = -M^{-1}\frac{\partial \rho_u(q,u,z)}{\partial u}$$

where q are the generalized coordinates, u are the generalized speeds, W is a joint map matrix and M is the mass matrix and ρ_u is the dynamic residual of the equations of motion, and z is $-M^{-1}\rho_u(q,u,0)$.

4. The method of claim 3 wherein said implicit integrator selecting step comprises an L-stable integrator.

5. A method of simulating the behavior of a physical system, comprising

modeling said physical system with a torsion angle, rigid multibody model, said model having equations of motion; and

integrating said equations of motion with an implicit integrator; said implicit integrator having an analytic Jacobian to obtain calculations of said behavior of said physical system.

6. The method of claim 5 wherein said analytic Jacobian is derived from an analytic Jacobian of the Residual Form of the equations of motion.

7. The method of claim 6 wherein said analytic Jacobian J comprises

$$J = \begin{pmatrix} \frac{\partial \dot{q}}{\partial q} & \frac{\partial \dot{q}}{\partial u} \\ \frac{\partial \dot{u}}{\partial q} & \frac{\partial \dot{u}}{\partial u} \end{pmatrix} \triangleq \begin{pmatrix} J_{qq} & J_{qu} \\ J_{uq} & J_{uu} \end{pmatrix}\text{; and}$$

$$J_{qq} = \frac{\partial \dot{q}}{\partial q} = \frac{\partial (Wu)}{\partial q} \quad \text{and} \quad J_{qu} = \frac{\partial \dot{q}}{\partial u} = W$$

$$J_{uq} = \frac{\partial \dot{u}}{\partial q} = -M^{-1}\frac{\partial \rho_u(q,u,z)}{\partial q} \quad \text{and} \quad J_{uu} = \frac{\partial \dot{u}}{\partial u} = -M^{-1}\frac{\partial \rho_u(q,u,z)}{\partial u}$$

where q are the generalized coordinates, u are the generalized speed, W is a joint map matrix and M is the mass matrix and ρ_u is the dynamic residual of the equations of motion, and z is $-M^{-1}\rho_u(q,u,0)$.

8. The method of claim 7 wherein said implicit integrator comprises an L-stable integrator.

9. Computer code for simulating the behavior of a molecule, said code comprising

a first module for a torsion angle, rigid multibody model of said molecule, said model having equations of motion; and

a second module for an implicit integrator to integrate said equations of motion with an analytic Jacobian to obtain calculations of said behavior of said molecule.

10. The computer code of claim 9 wherein said analytic Jacobian is derived from an analytic Jacobian of the Residual Form of the equations of motion.

11. The computer code of claim 10 wherein said analytic Jacobian J comprises

$$J = \begin{pmatrix} \frac{\partial \dot{q}}{\partial q} & \frac{\partial \dot{q}}{\partial u} \\ \frac{\partial \dot{u}}{\partial q} & \frac{\partial \dot{u}}{\partial u} \end{pmatrix} \triangleq \begin{pmatrix} J_{qq} & J_{qu} \\ J_{uq} & J_{uu} \end{pmatrix}; \text{ and}$$

$$J_{qq} = \frac{\partial \dot{q}}{\partial q} = \frac{\partial (Wu)}{\partial q} \text{ and } J_{qu} = \frac{\partial \dot{q}}{\partial u} = W$$

$$J_{uq} = \frac{\partial \dot{u}}{\partial q} = -M^{-1} \frac{\partial \rho_u(q,u,z)}{\partial q} \text{ and } J_{uu} = \frac{\partial \dot{u}}{\partial u} = -M^{-1} \frac{\partial \rho_u(q,u,z)}{\partial u}$$

where q are the generalized coordinates, u are the generalized speed, W is a joint map matrix and M is the mass matrix and ρ_u is the dynamic residual of the equations of motion, and z is $-M^{-1}\rho_u(q,u,0)$.

12. The computer code of claim 11 wherein said implicit integrator comprises an L-stable integrator.

13. Computer code for simulating the behavior of a physical system, said code comprising

a first module for a torsion angle, rigid multibody model of said system, said model having equations of motion; and

a second module for an implicit integrator to integrate said equations of motion with an analytic Jacobian to obtain calculations of said behavior of said system.

14. The computer code of claim 13 wherein said analytic Jacobian is derived from an analytic Jacobian of the Residual Form of the equations of motion.

15. The computer code of claim 14 wherein said analytic Jacobian J comprises

$$J = \begin{pmatrix} \frac{\partial \dot{q}}{\partial q} & \frac{\partial \dot{q}}{\partial u} \\ \frac{\partial \dot{u}}{\partial q} & \frac{\partial \dot{u}}{\partial u} \end{pmatrix} \triangleq \begin{pmatrix} J_{qq} & J_{qu} \\ J_{uq} & J_{uu} \end{pmatrix}; \text{ and}$$

$$J_{qq} = \frac{\partial \dot{q}}{\partial q} = \frac{\partial (Wu)}{\partial q} \text{ and } J_{qu} = \frac{\partial \dot{q}}{\partial u} = W$$

$$J_{uq} = \frac{\partial \dot{u}}{\partial q} = -M^{-1} \frac{\partial \rho_u(q,u,z)}{\partial q} \text{ and } J_{uu} = \frac{\partial \dot{u}}{\partial u} = -M^{-1} \frac{\partial \rho_u(q,u,z)}{\partial u}$$

where q are the generalized coordinates, u are the generalized speed, W is a joint map matrix and M is the mass matrix and ρ_u is the dynamic residual of the equations of motion, and z is $-M^{-1}\rho_u(q,u,0)$.

16. The computer code of claim 15 wherein said implicit integrator comprises an L-stable integrator.